

SEARCH REQUEST FORM

56031

Requestor's
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Gerstl

Serial
Number:

662457

Date:

12/4/01

Phone:

308 4531

Art Unit:

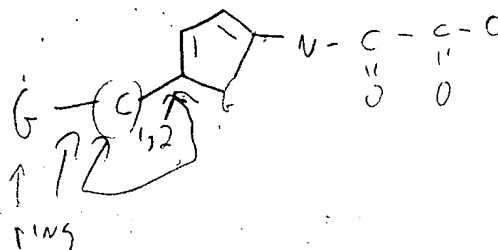
1626 3609

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Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).

G = O.S



Point of Contact:
Jan Delaval
Librarian, Physical Sciences
CM1 1E01 Tel: 308-4498

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☒ Structure
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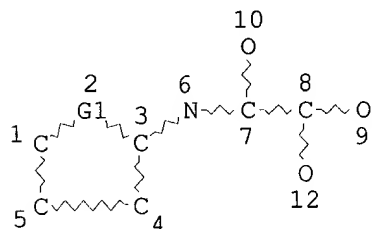
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 for more information. See STNote 27, Searching Properties in the CAS
 Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d sta que l11

L3 STR



VAR G1=O/S

NODE ATTRIBUTES:

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CONNECT IS M3 R AT 5

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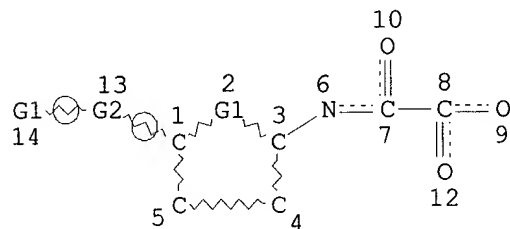
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STEREO ATTRIBUTES: NONE

L5 555 SEA FILE=REGISTRY SSS FUL L3

L6 STR



VAR G1=O/S

REP G2=(1-2) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

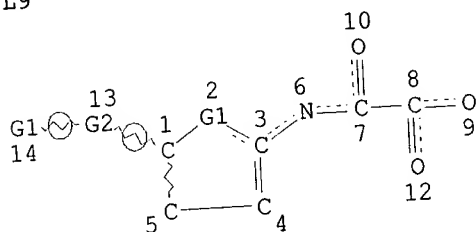
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

Point of Contact:
 Jan DeLavel
 Librarian-Physical Sciences
 CM1 1E07 Tel: 308-4498

gerstl - 09 / 662457

STEREO ATTRIBUTES: NONE
 L8 272 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
 L9 STR



VAR G1=O/S
 REP G2=(1-2) C
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
 L10 272 SEA FILE=REGISTRY SUB=L5 SSS FUL L9
 L11 272 SEA FILE=REGISTRY ABB=ON PLU=ON L8 OR L10

=> d his 113-

(FILE 'HCAOLD' ENTERED AT 11:00:19 ON 04 DEC 2001)
 L13 0 S L11

FILE 'HCAPLUS' ENTERED AT 11:00:34 ON 04 DEC 2001
 L14 6 S L11

FILE 'USPATFULL' ENTERED AT 11:00:43 ON 04 DEC 2001
 L15 0 S L11

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 FILE LAST UPDATED: 3 Dec 2001 (20011203/ED)

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=> d 114 bib abs hitrn fhitrstr tot

L14 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2001 ACS

AN 2001:208280 HCAPLUS

DN 134:252328

TI Preparation of 2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acids as protein tyrosine phosphatase inhibitors

IN Andersen, Henrik Sune; Hansen, Thomas Kruse; Lau, Jesper; Moller, Niels Peter Hundahl; Olsen, Ole Hvilsted; Axe, Frank Urban; Ge, Yu; Holsworth, Daniel Dale; Jones, Todd Kevin; Judge, Luke Milburn; Ripka, William Charles; Shapira, Barry Zvi; Uyeda, Roy Teruyuki

PA Novo Nordisk A/S, Den.; Ontogen Corporation

SO PCT Int. Appl., 147 pp.

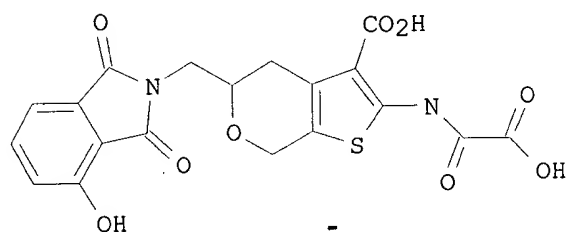
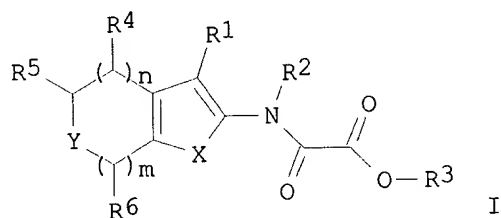
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001019831	A1	20010322	WO 2000-DK503	20000911
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
PRAI	DK 1999-1278	A	19990910		
OS	MARPAT 134:252328				
GI					



AB The title compds. (I) [wherein n = 0-2; m = 1 or 2; X = S or O; Y = O, S, SO, or SO2; R1 = H or CO2R3, tetrazolyl, 3-hydroxyoxazolyl, 3-hydroxyisothiazolyl, 3-hydroxypyrazolyl, 3-hydroxy-1,2,4-oxadiazolyl, 2-thio-1,3,4-oxadiazolyl, 2-hydroxyoxazolyl, 2-hydroxythiazolyl, etc.; R2 = H, alkyl, OH, or NR7R8; R3 = H (ar)alkyl, or alkylcarbonyloxy(ar)alkyl; R4-R6 = independently H, trihalomethyl, (ar)alkyl, (hetero)aryl, OH, oxo,

carboxy(alkyl), alkyloxycarbonyl, alkoxy(alkyl), (ar)alkyloxyalkyl, thio, alkylthio, (un)substituted amino, acyl, alkylcarbonylamino(alkyl), etc.; R7 and R8 = independently H, (ar)alkyl, aryl, (ar)alkylcarbonyl, arylcarbonyl, or (ar)alkylcarboxy; or R7 and R8 together with the N to which they are attached form an (un)substituted mono-, bi-, or tricyclic ring system contg. 0-3 heteroatoms; or R7 and R8 = independently a 5-7 membered amine, imide, or lactam] were prepd. as inhibitors of protein tyrosine phosphatases (PTPases), such as PTP1B, CD45, SHP-1, SHP-2, PTP.alpha., LAR, and HePTP. For example, 5-(4-benzyloxy-1,3-dioxo-1,3-dihydroisoindol-2-ylmethyl)-2-(tert-butoxyoxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid tert Bu ester was debenzylated using Pd/C in EtOAc (67%) and deesterified using 25% TFA in CH₂Cl₂ to afford II (72%). In a study evaluating for biol. activity against a truncated form of PTP1B, II inhibited PTP1B with a K_i of 1.5 .mu.M. I are useful in the treatment of type I diabetes, type II diabetes, impaired glucose tolerance, insulin resistance, obesity, and other diseases (no data).

IT 330192-16-0P 330192-18-2P 330192-20-6P
 330192-22-8P 330192-24-0P 330192-25-1P
 330192-27-3P 330192-30-8P 330192-31-9P
 330192-32-0P 330192-33-1P 330192-36-4P
 330192-38-6P 330192-39-7P 330192-41-1P
 330192-43-3P 330192-46-6P 330192-50-2P
 330192-52-4P 330192-53-5P 330192-55-7P
 330192-56-8P 330192-59-1P 330192-61-5P
 330192-63-7P 330192-68-2P 330192-71-7P
 330192-72-8P 330192-76-2P 330192-78-4P
 330192-81-9P 330192-82-0P 330192-84-2P
 330192-90-0P 330192-91-1P 330192-93-3P
 330193-42-5P 330193-46-9P 330193-47-0P
 330193-52-7P 330193-55-0P 330193-57-2P
 330193-58-3P 330653-63-9P 330653-65-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (intermediate; prepn. of 2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acids as PTP1B inhibitors for treatment of diabetes, impaired glucose tolerance, insulin resistance, obesity, and other diseases)

IT 330653-64-0P

RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acids as PTP1B inhibitors for treatment of diabetes, impaired glucose tolerance, insulin resistance, obesity, and other diseases)

IT 243967-61-5P 243967-62-6P 243967-63-7P
 243967-64-8P 243967-71-7P 243967-72-8P
 243967-73-9P 243967-74-0P 243967-75-1P
 243967-81-9P 330191-23-6P 330191-24-7P,
 7-(2,4-Dioxothiazolidin-3-ylmethyl)-2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid 330191-25-8P
 330191-26-9P 330191-27-0P 330191-28-1P
 330191-29-2P 330191-30-5P 330191-31-6P
 330191-32-7P 330191-33-8P 330191-34-9P,
 2-(Oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3,7-dicarboxylic acid 7-ethyl ester 330191-35-0P, 7-Benzylcarbonyl-2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid 330191-36-1P
 330191-37-2P 330191-38-3P 330191-39-4P
 330191-40-7P, 2-[[[3-Carboxy-2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-5-yl]methyl]carbonyl]nicotinic acid
 330191-41-8P 330191-43-0P 330191-44-1P
 330191-45-2P 330191-46-3P 330191-47-4P
 330191-48-5P, 7-[[5-(3,5-Dimethoxybenzylidene)-2,4-dioxothiazolidin-3-yl]methyl]-2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid 330191-49-6P 330191-50-9P
 330191-53-2P 330191-55-4P 330191-56-5P
 330191-57-6P 330191-58-7P 330191-59-8P

330192-23-9P 330192-28-4P 330192-69-3P,
 5-Benzylcarbamoyl-2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-
 carboxylic acid 330192-87-5P 330193-29-8P
 330193-30-1P 330193-31-2P 330193-32-3P
 330193-33-4P 330193-34-5P 330193-35-6P
 330193-36-7P 330193-37-8P 330193-38-9P
 330193-39-0P 330193-40-3P 330193-43-6P,
 2-(Oxalylamino)-5-(2,2,2-trifluoroacetoxymethyl)-4,7-dihydro-5H-thieno[2,3-
 c]pyran-3-carboxylic acid 330193-44-7P 330193-45-8P
 330193-48-1P 330193-49-2P 330193-50-5P
 330193-53-8P 330653-66-2P 330653-69-5P
 330653-71-9P 330653-72-0P 330653-73-1P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acids as PTP1B inhibitors for treatment of diabetes, impaired glucose tolerance, insulin resistance, obesity, and other diseases)

IT 243968-53-8 330192-17-1 330192-21-7
 330192-29-5 330192-85-3

RL: RCT (Reactant)

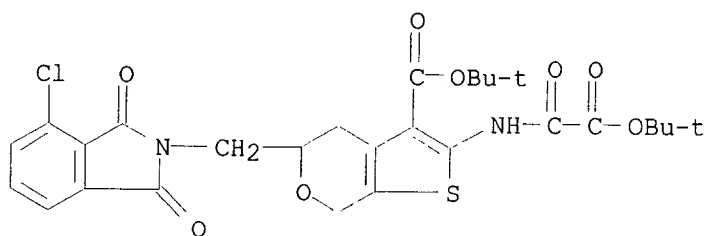
(reactant; prepn. of 2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acids as PTP1B inhibitors for treatment of diabetes, impaired glucose tolerance, insulin resistance, obesity, and other diseases)

IT 330192-16-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (intermediate; prepn. of 2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acids as PTP1B inhibitors for treatment of diabetes, impaired glucose tolerance, insulin resistance, obesity, and other diseases)

RN 330192-16-0 HCAPLUS

CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 5-[(4-chloro-1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-2-[[[(1,1-dimethylethoxy)oxoacetyl]amino]-4,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 7

RE

- (1) Bristol-Myers Company; GB 1583679 A 1981 HCAPLUS
 - (2) Iversen, L; The Journal of Biological Chemistry 2000, V275(14), P10300 HCAPLUS
 - (3) Novo Nordisk AS; WO 9946237 A1 1999 HCAPLUS
 - (4) Novo Nordisk AS; WO 9946267 A1 1999 HCAPLUS
 - (5) Novo Nordisk AS; WO 9946268 A1 1999 HCAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2001 ACS

AN 2001:185561 HCAPLUS

DN 134:237465

TI Method of inhibiting protein tyrosine phosphatases with an aspartic acid residue at position 48

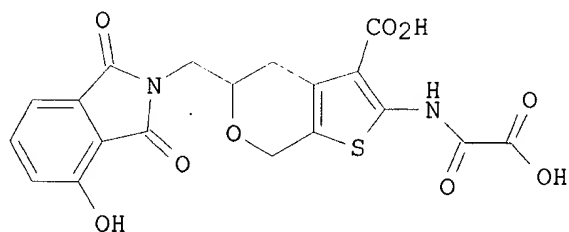
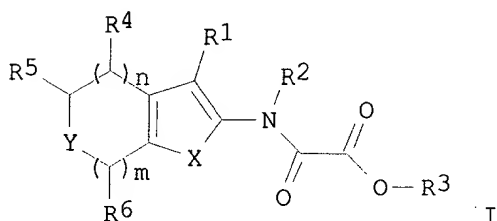
IN Andersen, Henrik Sune; Hansen, Thomas Kruse; Iverson, Lars Fogh; Lau, Jesper; Moller, Niels Peter Hundahl; Olsen, Ole Hvilsted; Axe, Frank Urban; Ge, Yu; Holsworth, Daniel Dale; Jones, Todd Kevin; Judge, Luke

Milburn; Ripka, William Charles; Shapira, Barry Zvi; Uyeda, Roy Teruyuki
 PA Novo Nordisk A/S, Den.; Ontogen Corp.
 SO PCT Int. Appl., 644 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001017516	A2	20010315	WO 2000-US24761	20000911
	WO 2001017516	A3	20011108		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
PRAI	DK 1999-1279	A	19990910		
	US 1999-156641	P	19990929		

GI

60/156



AB The present invention provides a method of inhibiting protein tyrosine phosphatases (PTPases, PTPs), such as PTP1B, TC-PTP, CD45, SHP-1, PTP.alpha., PTP.epsilon., PTP.beta., PTP D1, PTP D2, PTPH1, and PTP-LAR, by administration of compds. which have structural, phys., and spatial characteristics that allow them to interact with an aspartic acid residue at position 48 of PTP1B and/or TC-PTP. Prepns. for over 100 thieno[2,3-c]pyrans and thieno[2,3-c]pyridines (I) [wherein n = 0-2; m = 0-2; and m = n .gtoreq. 1; X = S, O, NR8; Y = NR8, O, S, SO, SO2; R1 = H, CO2R3, or a 5-membered heterocycle such as tetrazolyl, 3-hydroxyisoxazolyl, 3-hydroxyisothiazolyl, 3-hydroxypyrazolyl, 2-(hydroxy or thio)-1,3,4-oxadiazolyl, 2-oxoimidazolyl, etc.; R2 = H, alkyl, .OH, or NR9R10; R3 = H, (ar)alkyl, or alkylcarbonyloxy(ar)alkyl; R4 - R6 = independently H, trihalomethyl, (ar)alkyl, aryl, OH, oxo, CO2H, carboxyalkyl, (ar)alkyloxycarbonyl, alkylaminoalkyl, (ar)alkylcarbonylamino, etc.; R8 - R10 = independently H or (un)substituted (ar)alkyl, aryl, (ar)alkylcarbonyl, arylcarbonyl, or (ar)alkylcarboxy; or R9 and R10 together with the N to which they are attached form an (un)substituted cyclic, bicyclic, or tricyclic ring

system contg. 0-3 heteroatoms; or R9 and R10 = independently a 5-7 membered cyclic amine, imide, or lactam] and structural-based PTPase inhibition data are included. For example, 5-(4-benzyloxy-1,3-dioxo-1,3-dihydroisindol-2-ylmethyl)-2-(tert-butoxyoxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid tert-Bu ester was debenzylated using Pd/C and treated with 25% TFA in CH₂Cl₂ to give II. II showed potency against PTP1B, PTP.alpha. D1, PTP.epsilon. D1, PTP.beta., and CD45 D1D2 with K_i values (μ M) of 1.9, 93, 11, 1.1, and 130, resp. I are indicated in the management or treatment of a broad range of diseases such as autoimmune diseases, acute and chronic inflammation, osteoporosis, various forms of cancer and malignant diseases, and type I diabetes and type II diabetes (no data). In addn., I are useful in the isolation of PTPases and in elucidation of their biol. function.

IT 243967-73-9D, 5-(4-Hydroxy-1,3-dioxo-1,3-dihydroisindol-2-ylmethyl)-2-(oxalylamino)-4,7-dihydrothieno[2,3-c]pyran-3-carboxylic acid, complex with PTP1B 330191-26-9D, complex with PTP1B 330191-58-7D, complex with PTP1B
 RL: PRP (Properties)

(crystal structure of PTP1B complex with PTPase inhibitor)

IT 330192-16-0P 330192-18-2P 330192-20-6P
 330192-22-8P 330192-24-0P 330192-25-1P
 330192-27-3P 330192-30-8P 330192-31-9P
 330192-32-0P 330192-33-1P 330192-36-4P
 330192-38-6P 330192-39-7P 330192-41-1P
 330192-43-3P 330192-46-6P 330192-50-2P
 330192-51-3P 330192-52-4P 330192-53-5P
 330192-55-7P 330192-56-8P 330192-59-1P
 330192-61-5P 330192-63-7P 330192-68-2P
 330192-71-7P 330192-72-8P 330192-76-2P
 330192-78-4P 330192-81-9P 330192-82-0P
 330192-84-2P 330192-86-4P 330192-90-0P
 330192-91-1P 330192-93-3P 330193-42-5P
 330193-46-9P 330193-47-0P 330193-52-7P
 330193-55-0P 330193-57-2P 330193-58-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(intermediate; structure-based design and prepn. of selective inhibitors of protein tyrosine phosphatases)

IT 243968-53-8 330192-17-1 330192-21-7
 330192-29-5 330192-85-3

RL: RCT (Reactant)
 (reactant; structure-based design and prepn. of selective inhibitors of protein tyrosine phosphatases)

IT 243967-61-5P 243967-62-6P 243967-63-7P
 243967-64-8P 243967-71-7P 243967-72-8P
 243967-73-9P 243967-74-0P 243967-75-1P
 243967-81-9P 330191-23-6P 330191-24-7P
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 330193-53-8P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(structure-based design and prepn. of selective inhibitors of protein tyrosine phosphatases)

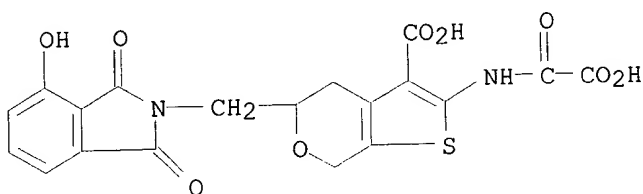
IT **243967-73-9D**, 5-(4-Hydroxy-1,3-dioxo-1,3-dihydroisoindol-2-ylmethyl)-2-(oxalylamino)-4,7-dihydrothieno[2,3-c]pyran-3-carboxylic acid, complex with PTP1B

RL: PRP (Properties)

(crystal structure of PTP1B complex with PTPase inhibitor)

RN 243967-73-9 HCAPLUS

CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-5-[(1,3-dihydro-4-hydroxy-1,3-dioxo-2H-isoindol-2-yl)methyl]-4,7-dihydro-(9CI) (CA INDEX NAME)



L14 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2001 ACS

AN 2000:438570 HCAPLUS

DN 133:219278

TI Residue 259 is a key determinant of substrate specificity of protein-tyrosine phosphatases 1B and .alpha.

AU Peters, Gunther H.; Iversen, Lars Fogh; Branner, Sven; Andersen, Henrik Sune; Mortensen, Steen B.; Olsen, Ole Hvilsted; Moller, Karin Bach; Moller, Niels Peter Hundahl

CS Department of Chemistry, Membrane and Statistical Physics Group (MEMPHYS), Technical University of Denmark, Lyngby, DK-2800, Den.

SO J. Biol. Chem. (2000), 275(24), 18201-18209
CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Biology

DT Journal

LA English

AB The aim of this study was to define the structural elements that det. the differences in substrate recognition capacity of two protein-tyrosine phosphatases (PTPs), PTP1B and PTP.alpha., both suggested to be neg. regulators of insulin signaling. Since the AcDADE(pY)L-NH2 peptide is well recognized by PTP1B, but less efficiently by PTP.alpha., it was chosen as a tool for these analyses. C.alpha. regiovariation analyses and primary sequence alignments indicate that residues 47, 48, 258, and 259 (PTP1B numbering) define a selectivity-detg. region. By analyzing a set of DADE(pY)L analogs with a series of PTP mutants in which these four residues were exchanged between PTP1B and PTP.alpha., either in combination or alone, we here demonstrate that the key selectivity-detg. residue is 259. In PTP.alpha., this residue is a glutamine causing steric hindrance and in PTP1B a glycine allowing broad substrate recognition. Significantly, replacing Gln259 with a glycine almost turns PTP.alpha. into a PTP1B-like enzyme. By using a novel set of PTP inhibitors and x-ray crystallog., we further provide evidence that Gln259 in PTP.alpha. plays a dual role leading to restricted substrate recognition (directly via steric hindrance) and reduced catalytic activity (indirectly via Gln262). Both effects may indicate that PTP.alpha. regulates highly selective signal transduction processes.

IT **243966-19-0**

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); BIOL (Biological study)

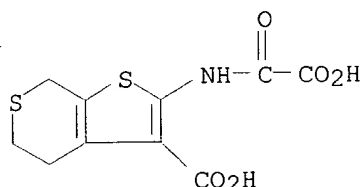
(reaction kinetics of peptides with protein-tyrosine phosphatases 1B and .alpha. wild-type and mutant forms and crystal structure studies of 1B isoenzyme)

IT 243966-19-0

RL: BAC (Biological activity or effector, except adverse); PRP
(Properties); BIOL (Biological study)
(reaction kinetics of peptides with protein-tyrosine phosphatases 1B
and .alpha. wild-type and mutant forms and crystal structure studies of
1B isoenzyme)

RN 243966-19-0 HCAPLUS

CN 5H-Thieno[2,3-c]thiopyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-
4,7-dihydro- (9CI) (CA INDEX NAME)



RE.CNT 46

RE

- (1) Andersen, H; J Biol Chem 2000, V275, P7101 HCAPLUS
 - (2) Barford, D; Science 1994, V263, P1397 HCAPLUS
 - (3) Bilwes, A; Nature 1996, V382, P555 HCAPLUS
 - (5) Burke, T; Biochemistry 1996, V35, P15989 HCAPLUS
 - (6) Burke, T; Biopolymers 1998, V47, P225 HCAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2001 ACS

AN 2000:251041 HCAPLUS

DN 133:70565

TI Structure-based design of a low molecular weight, nonphosphorus,
nonpeptide, and highly selective inhibitor of protein-tyrosine phosphatase
1B

AU Iversen, Lars Fogh; Andersen, Henrik Sune; Branner, Sven; Mortensen, Steen
B.; Peters, Gunther H.; Norris, Kjeld; Olsen, Ole Hvilsted; Jeppesen,
Claus Bekker; Lundt, Behrend F.; Ripka, William; Moller, Karin Bach;
Moller, Niels Peter Hundahl

CS Protein Chemistry, Bagsvaerd, DK-2880, Den.

SO J. Biol. Chem. (2000), 275(14), 10300-10307

CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Biology

DT Journal

LA English

AB Several protein-tyrosine phosphatases (PTPs) have been proposed to act as
neg. regulators of insulin signaling. Recent studies have shown increased
insulin sensitivity and resistance to obesity in PTP1B knockout mice, thus
pointing to this enzyme as a potential drug target in diabetes.
Structure-based design, guided by PTP mutants and x-ray protein
crystallog., was used to optimize a relatively weak, nonphosphorus,
nonpeptide general PTP inhibitor (2-(oxalyl-amino)-benzoic acid) into a
highly selective PTP1B inhibitor. This was achieved by addressing residue
48 as a selectivity detg. residue. By introducing a basic nitrogen in the
core structure of the inhibitor, a salt bridge was formed to Asp-48 in
PTP1B. In contrast, the basic nitrogen causes repulsion in other PTPs
contg. an asparagine in the equiv. position resulting in a remarkable
selectivity for PTP1B. Importantly, this was accomplished while retaining
the mol. wt. of the inhibitor below 300 g/mol.

IT 243967-41-1

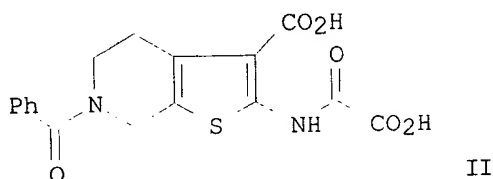
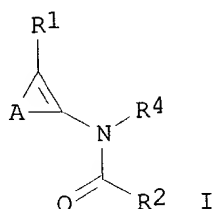
RL: BAC (Biological activity or effector, except adverse); PRP
(Properties); BIOL (Biological study)

(structure-based design of a low mol. wt., nonphosphorus, nonpeptide,
and highly selective inhibitor of protein-tyrosine phosphatase 1B)

IT 243967-41-1D, complexes with protein-tyrosine phosphatase 1B

RL: PRP (Properties)

DK 1998-938 A 19980715
 DK 1998-1385 A 19981028
 DK 1998-1612 A 19981207
 US 1998-82915 P 19980424
 US 1998-93525 P 19980721
 US 1998-108747 P 19981117
 WO 1999-DK121 W 19990311
 OS MARPAT 131:243258
 GI



AB Thieno[2,3-c]pyrans and thieno[2,3-c]pyridines (I) [A = atoms to complete various 5/5 and 5/6 bicyclic heterocycles, e.g., thienopridines, thieno(thio)pyrans, benzothiophenes, etc.; R1 and R2 = independently acyl, OH or derivs., CF3, NO2, cyano, SO3H, (un)substituted NH2 or PO3H2, or various 5-membered heterocycles; R4 = H, OH, alkyl, (un)substituted aryl or aralkyl, (un)substituted NH2, alkoxy] were prep'd. as inhibitors of Protein Tyrosine Phosphatases (PTPases) such as PTP1B, CD45, SHP-1, SHP-2, PTP.alpha., LAR, and HePTP. The compds. are useful in the treatment of type I diabetes, type II diabetes, impaired glucose tolerance, insulin resistance, obesity, immune dysfunctions including autoimmunity diseases with dysfunctions of the coagulation system, allergic diseases including asthma, osteoporosis, proliferative disorders including cancer and psoriasis, diseases with decreased or increased synthesis or effects of growth hormone, diseases with decreased or increased synthesis of hormones or cytokines that regulate the release of/or response to growth hormone, diseases of the brain including Alzheimer's disease and schizophrenia, and infectious diseases. For instance, 2-amino-6-benzoyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylic acid Et ester was amidated with Et oxalyl chloride in THF (84%), followed by hydrolysis of the ester function with NaOH in aq. soln. to give the title compd.(II) as the mono-Na salt (III) in 79% yield. In an in vitro test against PTP1B expressed in E. coli and purified by known methods, III had a Ki of 51 .mu.M.

IT 243968-05-0P 243968-12-9P 243968-16-3P
 243968-17-4P 243968-19-6P 243968-22-1P
 243968-28-7P 243968-33-4P 243968-35-6P
 243968-42-5P 243968-45-8P 243968-48-1DP, Wang
 resin-bound

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (intermediate; prepn. of thieno[2,3-c]pyrans and thieno[2,3-c]pyridines
 as modulators of protein tyrosine phosphatases (PTPases))

IT 243968-53-8 243968-54-9
 RL: RCT (Reactant)

(reactant; prepn. of thieno[2,3-c]pyrans and thieno[2,3-c]pyridines as
 modulators of protein tyrosine phosphatases (PTPases))

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 243966-40-7P 243966-42-9P 243966-43-0P
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243967-86-4P 243967-87-5P 243967-88-6P
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243967-92-2P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

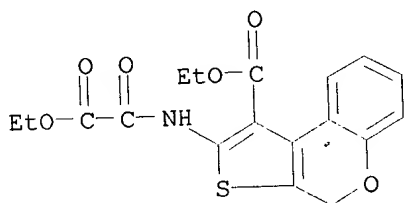
(target compd.; prepn. of thieno[2,3-c]pyrans and thieno[2,3-c]pyridines as modulators of protein tyrosine phosphatases (PTPases))

IT 243968-05-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (intermediate; prepn. of thieno[2,3-c]pyrans and thieno[2,3-c]pyridines as modulators of protein tyrosine phosphatases (PTPases))

RN 243968-05-0 HCAPLUS

CN 4H-Thieno[2,3-c][1]benzopyran-1-carboxylic acid, 2-[(ethoxyoxoacetyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



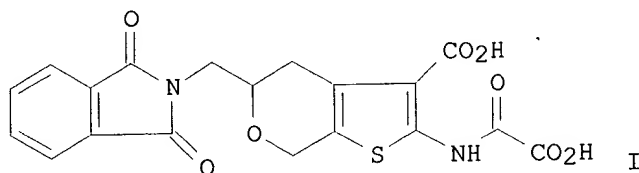
RE.CNT 8

RE

(1) AS Ferrosan; EP 0348872 A1 1990 HCAPLUS
(2) Basf Ag; DE 3112164 A1 1982 HCAPLUS

US 1998-93525	P	19980721
US 1998-93638	P	19980721
US 1998-108747	P	19981117
WO 1999-DK126	W	19990312

GI



AB Oxalylaminoheterocycles (e.g., oxalylaminothiophene and oxalylaminothienopyran derivs., etc.) were prep'd. as inhibitors of Protein Tyrosine Phosphatases (PTPases), such as PTP1B, TC-PTP, CD45, SHP-1, SHP-2, PTP.alpha., PTP.epsilon., PTP.mu., PTP.delta., PTP.sigma., PTP.zeta., PTP.beta., PTPD1, PTPD2, PTPH1, PTP-MEG1, PTP-LAR, and HePTP. These compds. are indicated in the management or treatment of a broad range of diseases such as autoimmune diseases, acute and chronic inflammation, osteoporosis, various forms of cancer and malignant diseases, and type I diabetes and type II diabetes. For instance, 2-amino-5-hydroxymethyl-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid tert-Bu ester (prepn. given) was reacted with phthalimide in THF, PPh3, and DIAD to form the 5-phthalimidomethyl deriv. (47%). The amine was amidated with imidazol-1-yloxoacetic acid tert-Bu ester in CH2Cl2 and TEA (99%), followed by hydrolysis of the ester function with TFA in CH2Cl2, to give 5-(1,3-dioxo-1,3-dihydroisoindol-2-ylmethyl)-2-(oxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid (I) in 57% yield. In an in vitro test against PTP1B expressed in E. coli and purified by known methods, Ki values at various inhibitor concns. were detd. An anal. of selectivity of two PTPase inhibitors against PTP1B, PTP-LAR, PTP.epsilon., CD45, and PTP.beta. showed that one compd. of the invention is a non-selective inhibitor, whereas another behaves like a selective inhibitor.

IT 243968-05-0P 243968-12-9P 243968-16-3P
 243968-17-4P 243968-19-6P 243968-22-1P
 243968-28-7P 243968-33-4P 243968-35-6P
 243968-42-5P 243968-45-8P 243968-48-1DP, Wang
 resin-bound

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (intermediate; prepn. of oxalylaminothiophene derivs. as modulators of
 protein tyrosine phosphatases (PTPases))

IT 243966-65-6P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
 preparation); THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); USES (Uses)
 (prepn. of oxalylaminothiophene derivs. as modulators of protein
 tyrosine phosphatases (PTPases))

IT 243968-53-8 243968-54-9 244014-84-4
 RL: RCT (Reactant)
 (reactant; prepn. of oxalylaminothiophene derivs. as modulators of
 protein tyrosine phosphatases (PTPases))

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RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

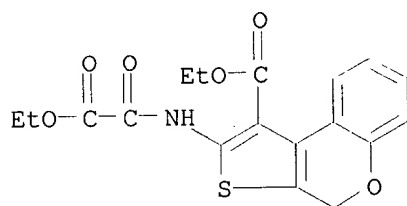
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IT 243968-05-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (intermediate; prepn. of oxalylaminothiophene derivs. as modulators of protein tyrosine phosphatases (PTPases))

RN 243968-05-0 HCAPLUS

CN 4H-Thieno[2,3-c][1]benzopyran-1-carboxylic acid, 2-
[(ethoxyoxoacetyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 2

RE

- (1) Geissler, J; Cancer research 1992, V52(16), P4492 HCAPLUS
- (2) Sugen, Inc; WO 9640113 A2 1996 HCAPLUS

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TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

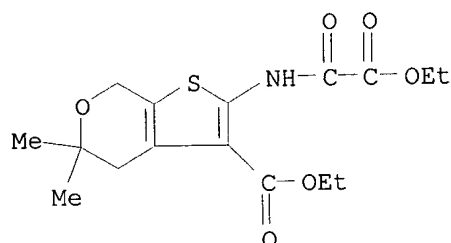
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

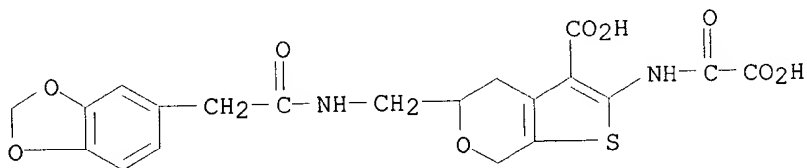
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L11 ANSWER 1 OF 272 REGISTRY COPYRIGHT 2001 ACS
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 FS 3D CONCORD
 MF C16 H21 N O6 S
 SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 ANSWER 15 OF 272 REGISTRY COPYRIGHT 2001 ACS
 RN 330193-50-5 REGISTRY
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 FS 3D CONCORD
 MF C20 H18 N2 O9 S
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER



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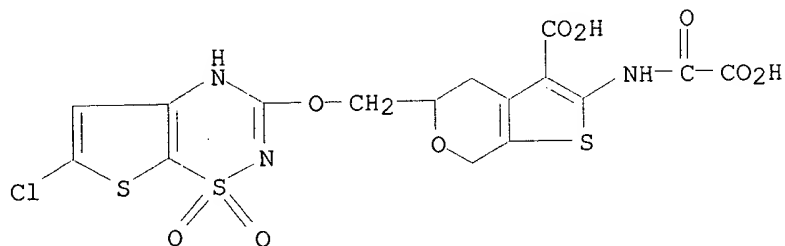
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 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:252328

REFERENCE 2: 134:237465

L11 ANSWER 30 OF 272 REGISTRY COPYRIGHT 2001 ACS

RN 330193-34-5 REGISTRY
 CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-5-[[6-chloro-1,1-dioxido-2H-thieno[3,2-e]-1,2,4-thiadiazin-3-yl)oxy]methyl]-4,7-dihydro- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C16 H12 Cl N3 O9 S3
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:252328

REFERENCE 2: 134:237465

L11 ANSWER 45 OF 272 REGISTRY COPYRIGHT 2001 ACS

RN 330192-78-4 REGISTRY

CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[[[(1,1-dimethylethoxy)oxoacetyl]amino]-4,7-dihydro-7-[[[4-(methylsulfonyl)phenyl]acetyl]amino]methyl]-, 1,1-dimethylethyl-ester- (9CI) (CA INDEX NAME)

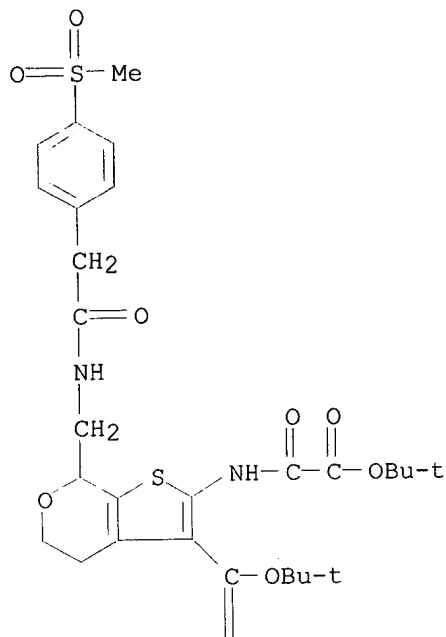
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MF C28 H36 N2 O9 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

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PAGE 2-A



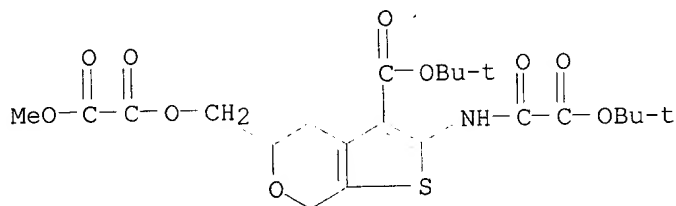
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2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:252328

REFERENCE 2: 134:237465

L11 ANSWER 60 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 330192-46-6 REGISTRY
CN Ethanedioic acid, [3-[(1,1-dimethylethoxy)carbonyl]-2-[[[(1,1-dimethylethoxy)oxoacetyl]amino]-4,7-dihydro-5H-thieno[2,3-c]pyran-5-yl]methyl methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H29 N O10 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:252328

REFERENCE 2: 134:237465

L11 ANSWER 75 OF 272 REGISTRY COPYRIGHT 2001 ACS

RN 330192-23-9 REGISTRY

CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-5-
[[1,3-dihydro-1,3-dioxo-4-(phenylmethoxy)-2H-isoindol-2-yl)methyl]-4,7-
dihydro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

MF C26 H20 N2 O9 S . C2 H F3 O2

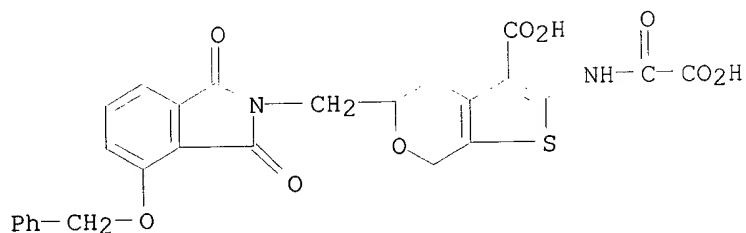
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

CM 1

CRN 330191-42-9

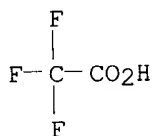
CMF C26 H20 N2 O9 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:252328

REFERENCE 2: 134:237465

L11 ANSWER 90 OF 272 REGISTRY COPYRIGHT 2001 ACS

RN 330191-51-0 REGISTRY

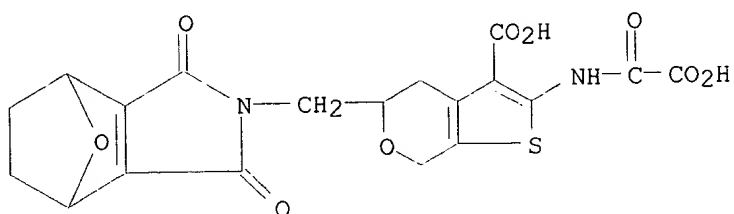
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-5-
[(1,3,4,5,6,7-hexahydro-1,3-dioxo-4,7-epoxy-2H-isoindol-2-yl)methyl]-4,7-
dihydro- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H16 N2 O9 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

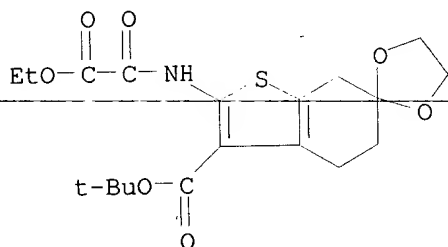


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:237465

L11 ANSWER 120 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243968-54-9 REGISTRY
CN Spiro[benzo[b]thiophene-6(5H), 2'-[1,3]dioxolane]-3-carboxylic acid,
2-[(ethoxyoxoacetyl)amino]-4,7-dihydro-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C19 H25 N O7 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



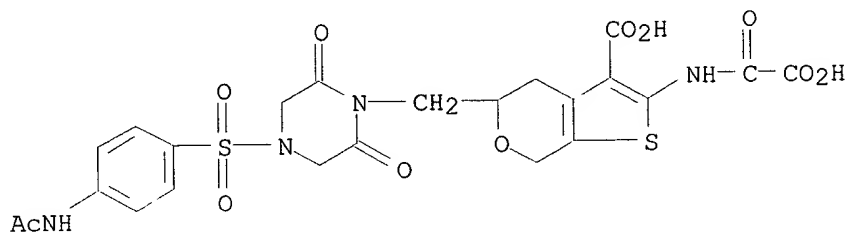
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643

L11 ANSWER 135 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243967-91-1 REGISTRY
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 5-[[4-[[4-(acetylamino)phenyl]sulfonyl]-2,6-dioxo-1-piperazinyl]methyl]-2-[(carboxycarbonyl)amino]-4,7-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H22 N4 O11 S2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

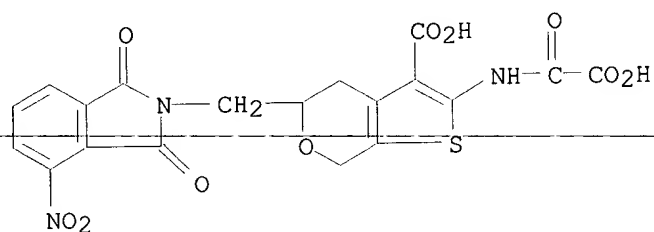


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

L11 ANSWER 150 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243967-75-1 REGISTRY
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-5-
[(1,3-dihydro-4-nitro-1,3-dioxo-2H-isoindol-2-yl)methyl]-4,7-dihydro-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H13 N3 O10 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

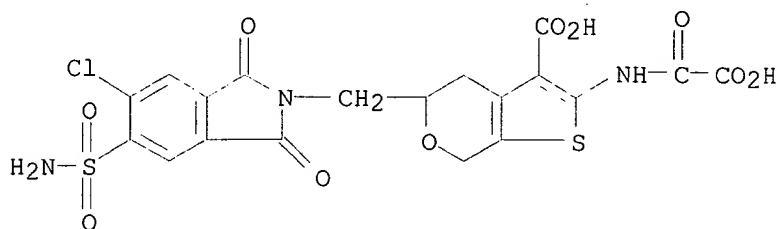
3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:252328

REFERENCE 2: 134:237465

REFERENCE 3: 131:243258

L11 ANSWER 165 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243967-60-4 REGISTRY
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 5-[[5-(aminosulfonyl)-6-chloro-
1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-2-[(carboxycarbonyl)amino]-
4,7-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H14 Cl N3 O10 S2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

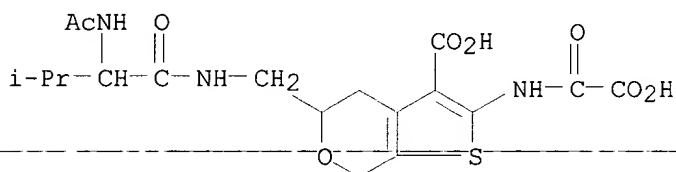


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

L11 ANSWER 180 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243967-30-8 REGISTRY
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 5-[[[2-(acetylamino)-3-methyl-1-oxobutyl]amino]methyl]-2-[(carboxycarbonylamino)amino]-4,7-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H23 N3 O8 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



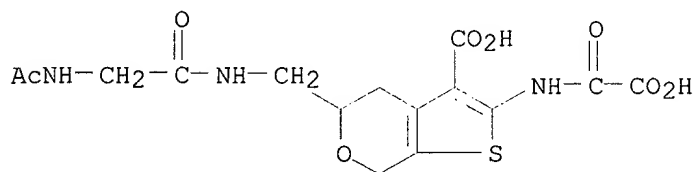
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643

L11 ANSWER 195 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243967-13-7 REGISTRY
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 5-[[[2-(acetylamino)acetyl]amino]methyl]-2-[(carboxycarbonylamino)amino]-4,7-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H17 N3 O8 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



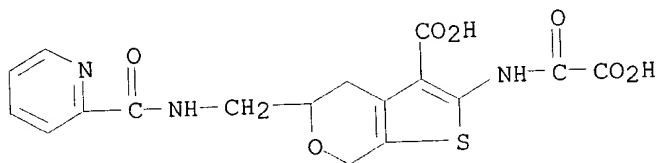
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643

L11 ANSWER 210 OF 272 'REGISTRY' COPYRIGHT 2001 ACS
RN 243966-92-9 'REGISTRY'
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-4,7-
dihydro-5-[[2-pyridinylcarbonyl)amino]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 N3 O7 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



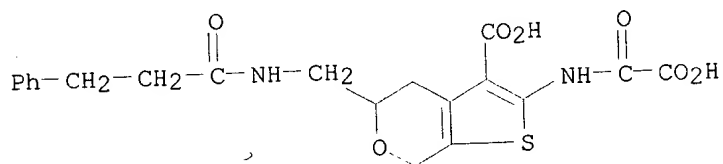
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643

L11 ANSWER 225 OF 272 'REGISTRY' COPYRIGHT 2001 ACS
RN 243966-75-8 'REGISTRY'
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-4,7-
dihydro-5-[[1-oxo-3-phenylpropyl)amino]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H20 N2 O7 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



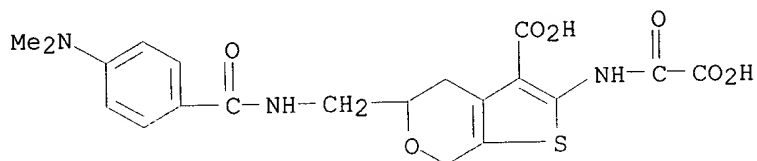
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643

L11 ANSWER 240 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243966-60-1 REGISTRY
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-5-[[4-(dimethylamino)benzoyl]amino]methyl]-4,7-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H21 N3 O7 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



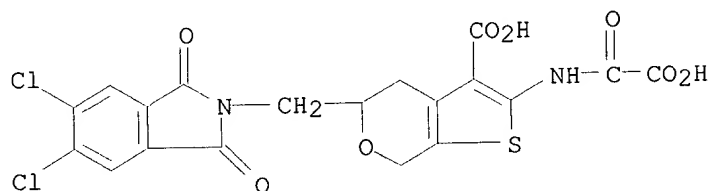
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643

L11 ANSWER 255 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243966-43-0 REGISTRY
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-5-[[5,6-dichloro-1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl]methyl]-4,7-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H12 Cl2 N2 O8 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



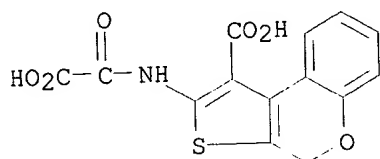
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643

L11 ANSWER 270 OF 272 REGISTRY COPYRIGHT 2001 ACS
RN 243966-20-3 REGISTRY
CN 4H-Thieno[2,3-c][1]benzopyran-1-carboxylic acid, 2-[(carboxycarbonyl)amino]-, monosodium salt (9CI) (CA INDEX NAME)
MF C14 H9 N O6 S . Na
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
CRN (243967-49-9)



● Na

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643

L11 ANSWER 272 OF 272 REGISTRY COPYRIGHT 2001 ACS

RN 243966-06-5 REGISTRY

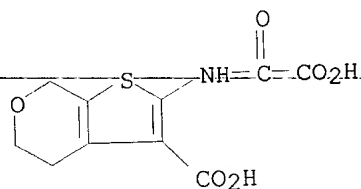
CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 2-[(carboxycarbonyl)amino]-4,7-dihydro-, monosodium salt (9CI) (CA INDEX NAME)

MF C10 H9 N O6 S . Na

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

CRN (243967-41-1)



● Na

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:243258

REFERENCE 2: 131:228643